Supplementary File S6

Pharmacophore Modeling of Top Ligand-Receptor Complexes

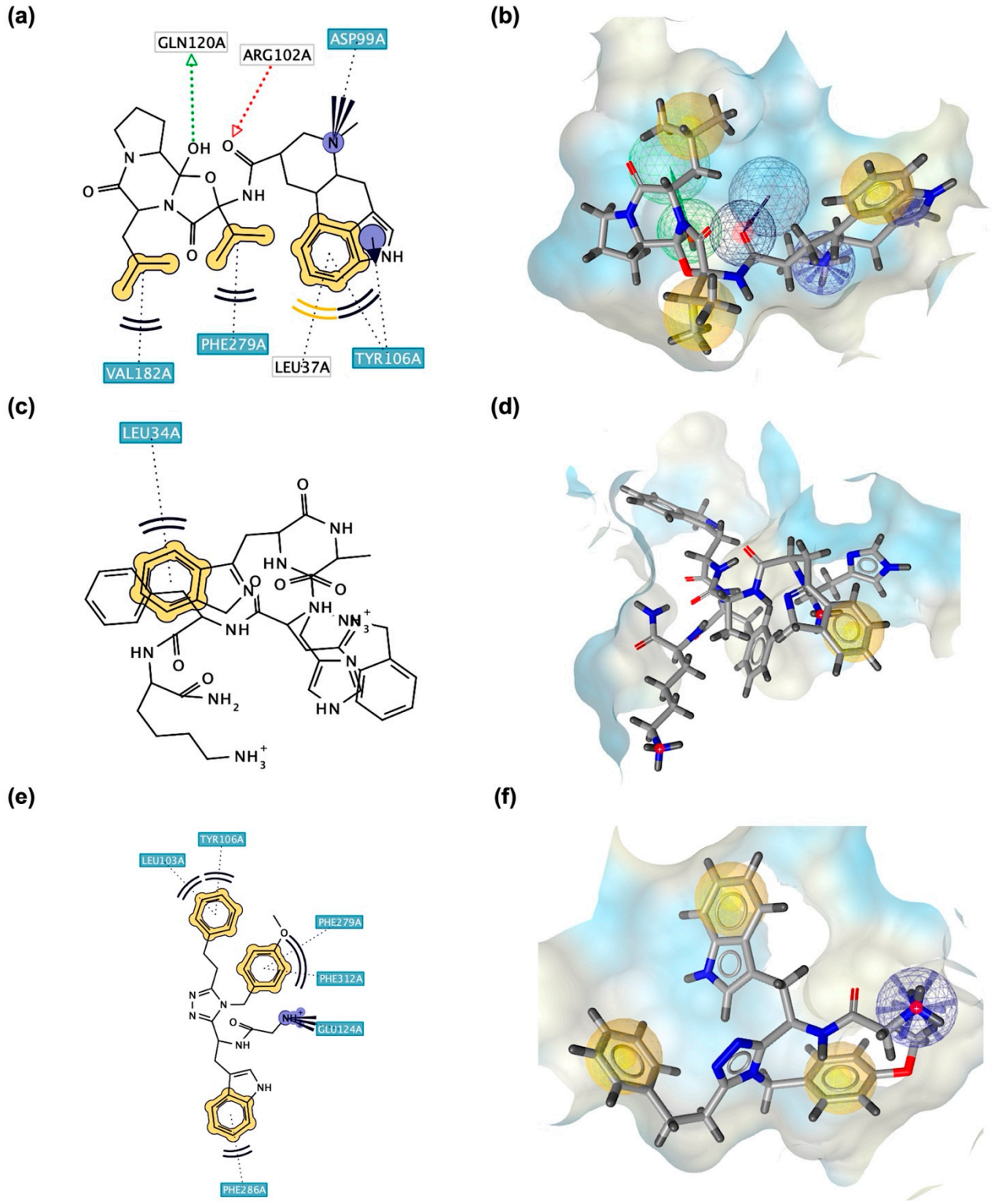


Figure S3. Pharmacophore modeling results of bromocriptine, standard agonists, and antagonists in the GHSR LBD. (**a**) 2D pharmacophore model of GHSR_Bromocriptine. (**b**) 3D pharmacophore model of GHSR_Bromocriptine. (**c**) 2D pharmacophore model of GHSR_GHRP-6 (agonist). (**d**) 3D pharmacophore model of GHSR_GHRP-6 (agonist). (**e**) 2D pharmacophore model of GHSR_JMV-2959 (antagonist). (**f**) 3D pharmacophore model of GHSR_JMV-2959 (antagonist). Yellow spheres indicate hydrophobic interactions, green arrows represent hydrogen bond donors, red arrows signify hydrogen bond acceptors, and blue stars represent a positive ionizable group.

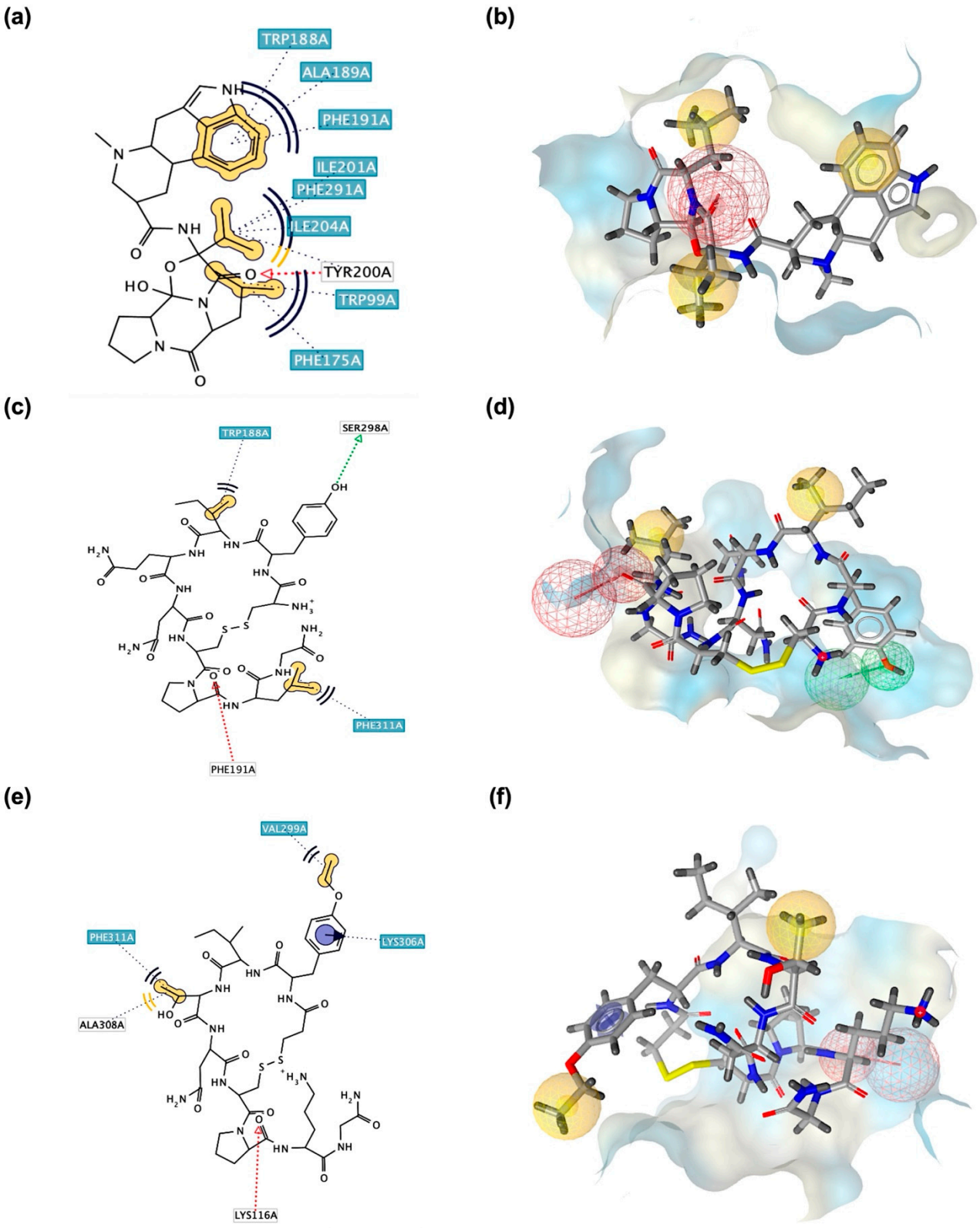


Figure S4. Pharmacophore modeling results of bromocriptine, standard agonists, and antagonists in the OXTR LBD. (**a**) 2D pharmacophore model of OXTR_Bromocriptine. (**b**) 3D pharmacophore model of OXTR_Bromocriptine. (**c**) 2D pharmacophore model of OXTR_Oxytocin (agonist). (**d**) 3D pharmacophore model of OXTR_Oxytocin (agonist). (**e**) 2D pharmacophore model of OXTR_Atosiban (antagonist). (**f**) 3D pharmacophore model of OXTR_Atosiban (antagonist).

Yellow spheres indicate hydrophobic interactions, green arrows represent hydrogen bond donors, red arrows signify hydrogen bond acceptors, and blue stars represent a positive ionizable group.